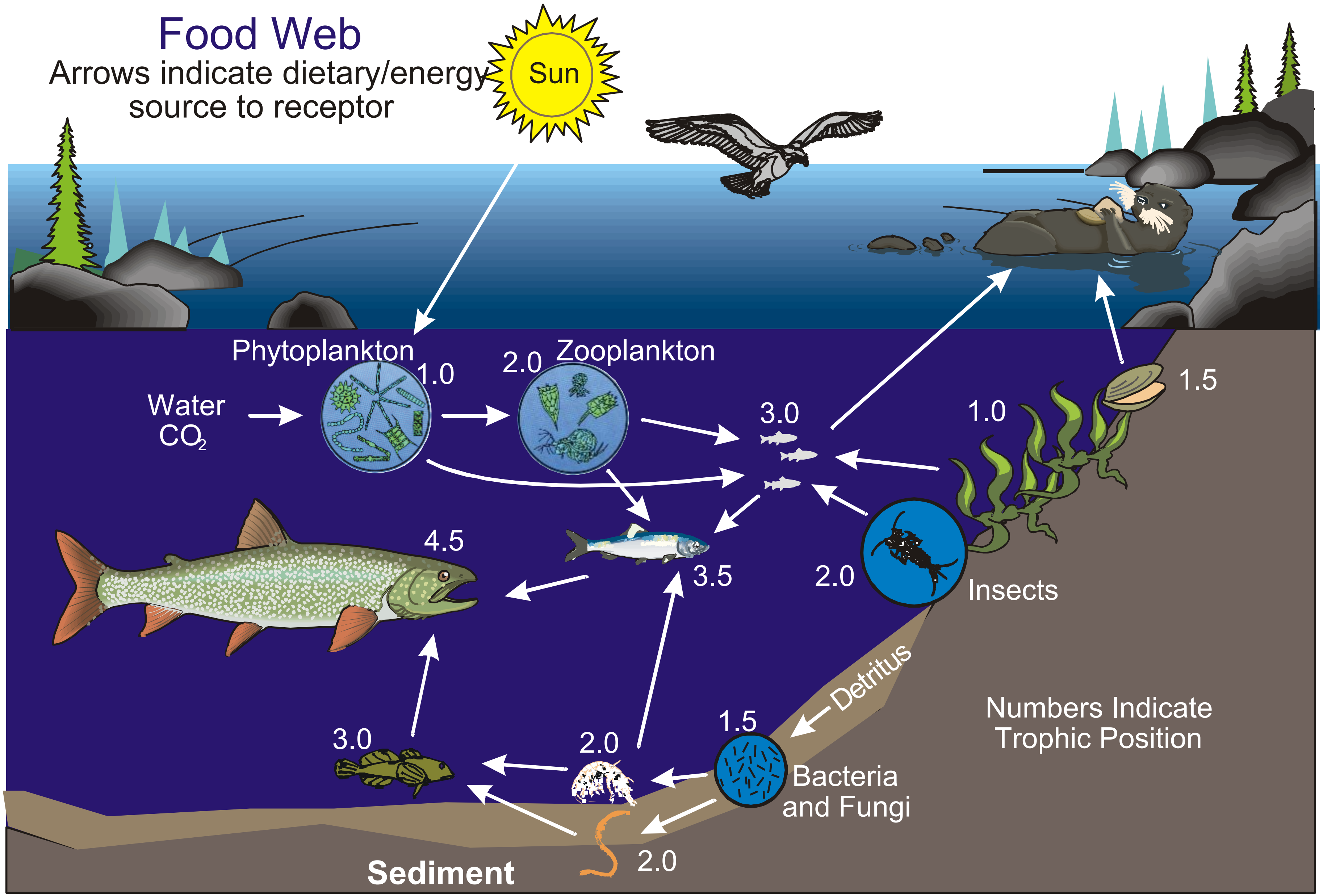
Predicting Chemical Residues in Aquatic Food Chains

Lawrence Burkhard
US-EPA, ORD, NHEERL, MED
Duluth, MN



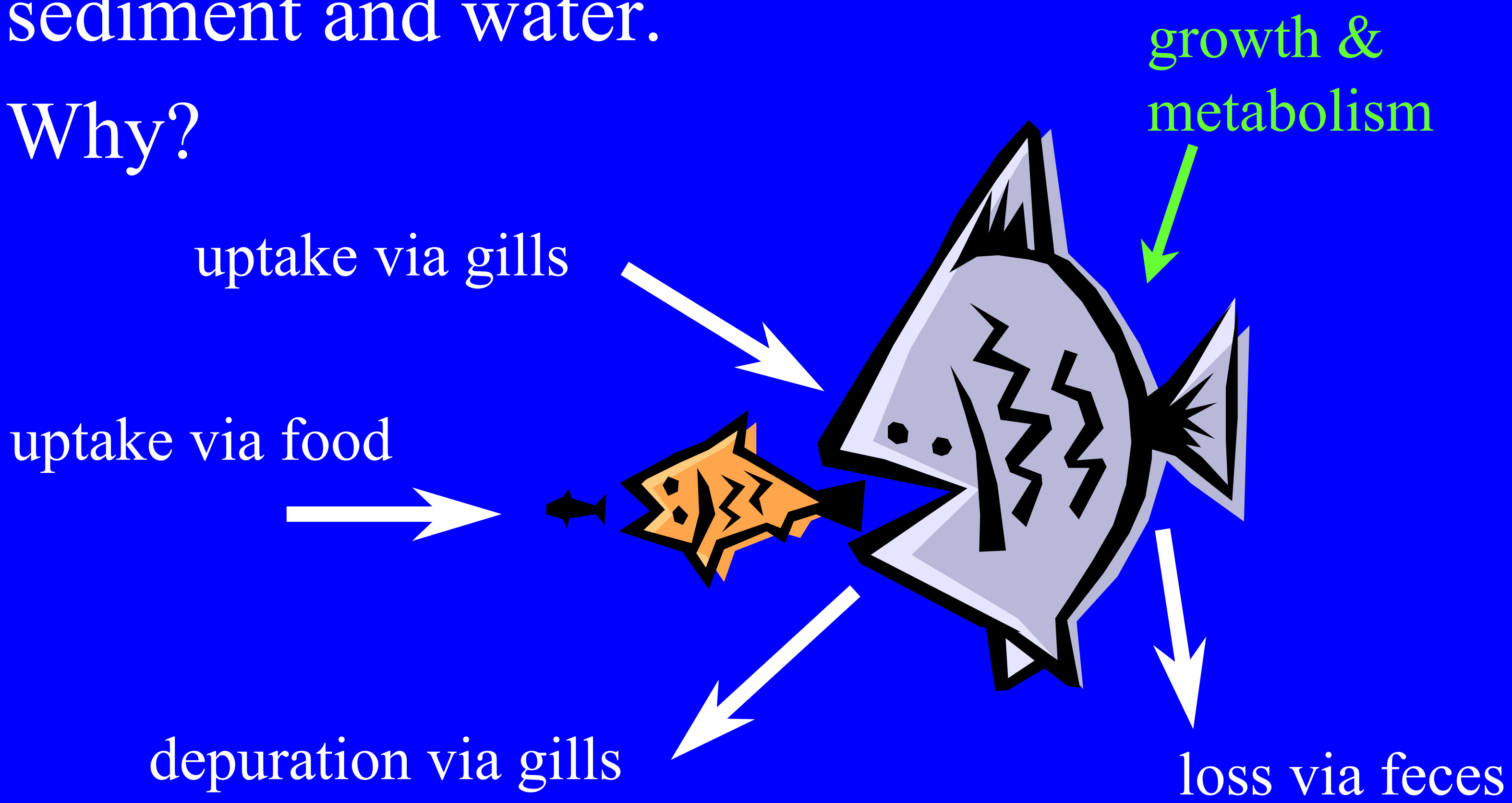
Food Web
Arrows indicate dietary/energy source to receptor
Sun
Phytoplankton
1.0
2.0
Zooplankton
Water
CO_2
3.0
1.0
1.5
4.5
3.5
2.0
Insects
Detritus
Numbers Indicate Trophic Position
1.5
3.0
2.0
Bacteria and Fungi
2.0
Sediment

General Problem

- How to quantitatively relate chemical concentrations in water and sediment to residues in fish?
- How to quantitatively relate chemical concentrations in benthic invertebrates to residues in fish?

Chemical Residues in Fish

- Function of both chemical concentrations in sediment and water.
- Why?



Chemical Residues in Fish

- Bioaccumulation Expressions
  - Sediment basis BSAF= C_{lipid} / C_{soc}
  - Water basis BAF_l^{fd}= C_{lipid} / C_w^{fd}
- BSAF & BAF_l^{fd} must be self consistent
  - predict the same chemical residue in fish

Chemical Residues in Fish

- BSAF predictions don't ignore water contamination
- BAF^{fd}_{l} predictions don't ignore sediment contamination
- Why?
    - Sediment and water column phases are interconnected in an ecosystem
        - fate and transport processes: hydrodynamics, diffusion, particle deposition & resuspension …

Approaches to Predicting Chemical Residues in Fish

- Empirical
  - field measured BSAFs or BAF_l^{fd}s
- Mechanistic
  - food chain models
- Empirical and mechanistic approaches:
  - compatible which each other
  - one can be used to support the other

Empirical Methods

- Incorporates all bioaccumulation processes
  - trophic transfer, metabolism, sediment-column water disequilibrium, bioavailability, organism growth, ...
- Ecosystem specific
  - incorporates existing loading scenario and contaminant burdens in sediments

Mechanistic Methods

- Many food chain models
  - Thomann
  - Gobas
  - Mackay (fugacity models)
  - Aquatox
  - Bass
  - ...

Mechanistic Models

- For each organism:

$$dC_f/dt = C_w\, k_1 + k_d \sum_{i}^{n} C_{di}\, f_i$$
$$- (k_2 + k_f + k_m + k_g)\, C_f$$

- Series of differential equations

Mechanistic Methods

- Steady-state solution $\mathbf{dC_f/dt = 0}$
  - long term
- Time dependent solution
  - chemical concentrations in water and sediment change over time
  - used in evaluating remediation options

Mechanistic Methods

- All models require:
  - – Ecosystem conditions
    - chemical concentrations in water & sediment, temperature, DOC, POC, SOC
  - – food chain structure
  - – organism specific parameters
    - weights, lipid contents, growth rates, *in vivo* metabolism rates, diets, migration/movement, ...
  - – chemical specific parameters: K_{ow}

Mechanistic Models

- All models require calibration for site specific predictions
- Inputs: data intensive
    - some models require more than others
- Outputs: dependent upon input quality

Mechanistic Models

- Primary drivers in model sensitivity and uncertainty
  - growth rate
  - lipids
  - plankton assimilation efficiencies
  - diet
  - disequilbrium
  - metabolism

Mechanistic Models

- Factors influencing forecasting results
  - quality of time-variant chemical concentrations in sediment and water
    - results from fate and transport models
  - consistency of food web structure
  - no major inputs or changes in loadings

Mechanistic Models

- Gobas-Thomann comparison (steady-state)
  - 90th/10th percentile predicted BAF^{fd}s
    - Gobas 3.6 Thomann [1] 4.0
  - measured-predicted BAF^{fd}s 4x
    - Gobas 89% Thomann 85%
- Morrison (steady-state)
  - measured-predicted BAF^{fd}s
    - Lake Ontario 2x-89% 10x-100%
    - Lake Erie (lake trout) 2x-62% 10x-90%

Mechanistic Models

- time-variant chemical concentrations
  - Hudson River
    - Connolly et al. 92% within 2x
    - FISHRAND 98% within 2x

Summary

- Two approaches to predicting residues
  – empirical and mechanistic
- Mechanistic models well developed
  – many models with similar predictive power
  – prediction accuracy of 2x
- Forecasts only as good as the input data
- Special considerations:
    - Metabolism & log K_{ow}s > 7.5